University of California
Lawrence Livermore National Laboratory

CASC Center for Applied Scientific Computing

Enabling Computational Technologies for Tera-Scale Simulations

Mission

We conduct collaborative scientific investigations which require the power of high performance computers and the efficiency of modern computational methods. Our research and development activities are applications driven, and focused on LLNL programmatic objectives that require advanced computational technologies. Our core competencies include high performance computing, numerical mathematics, computational physics, algorithm development, and scientific data management and visualization.

The Center for Applied Scientific Computing (CASC) at LLNL was formed in March 1996 as a focal point for computational science research and advanced applications development within the Computation Directorate. The nearly thirty numerical mathematicians, computational physicists, and computer scientists in CASC work closely with our colleagues in Livermore Computing (LC) and in Laboratory programs to enable tera-scale scientific simulations in a variety of application areas.

Computational Science Research Group

The Computational Science Research Group (CSR) develops new scientific application codes for high performance computers, and uses these codes to conduct collaborative, multidisciplinary scientific investigations. The design, implementation, and evaluation of new computational technologies are critical to the success of these efforts. The CSR works closely with the Advanced Applications Development Group to insure that these technologies are transferred to LLNL programs.

Advanced Applications Development Group

The Advanced Applications Development (AAD) Group works closely with LLNL programs (often as members of their code teams) to develop and port challenging scientific application codes to high performance computers. It also incorporates new computational technologies into these codes and develops scientific visualization software for the applications. The AAD collaborates with the CSR to insure that relevant research results are transferred to LLNL programs.

Collaborative Scientific Investigations

CASC is collaborating with several LLNL programs on applications in defense, energy, engineering, and environmental sciences. For example, we are numerically exploring materials properties (Figure 1) and turbulent flow (Figure 2) in support of the Laboratory's stockpile stewardship mission (ASCI). We are part of the Numerical Tokamak Project (Figure 3) for magnetic fusion energy and we are working with the oil industry to apply our expertise in neutron transport to nuclear well logging (Figure 4). We are building complex simulation codes to study environmental issues via global climate modeling (Figure 5) and subsurface flow and transport (Figure 6). Each of these collaborative scientific

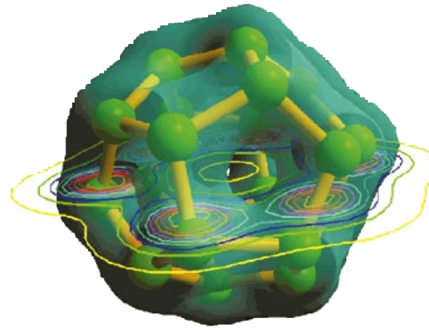

Fig. 1. Materials design seeks to understand materials properties through computer simulation.

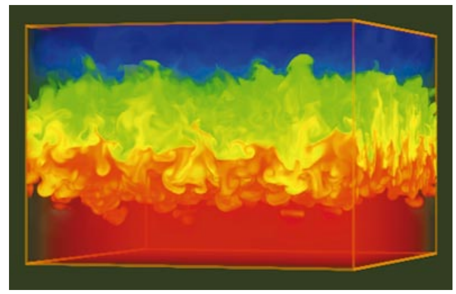

Fig. 2. Rayleigh-Taylor instability occurs when a light fluid attempts to support a heavier fluid.

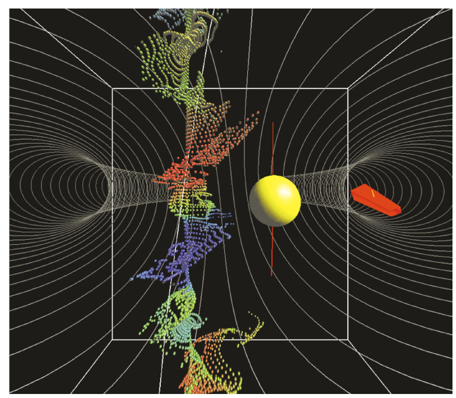

Fig. 3. Turbulent Gyro-Landau flow within a tokamak reactor (image taken from an interactive distributed visualization system).

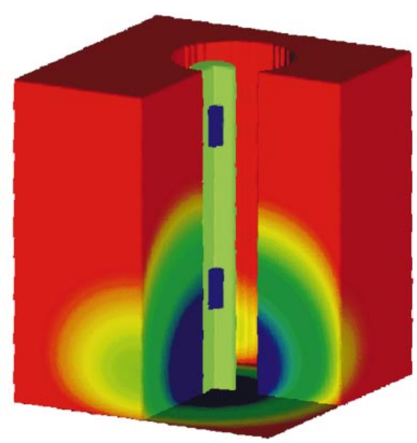

Fig. 4. Solution to a nuclear well logging problem for a water-filled borehole, using our new method for eliminating ray effects.

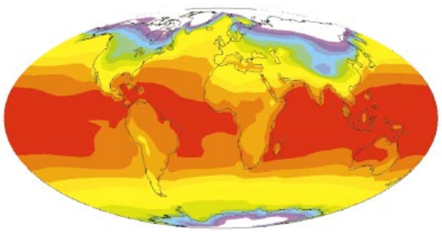

Fig. 5. Mean surface temperature during the Northern Hemisphere's winter months, as computed by our atmospheric general circulation model.

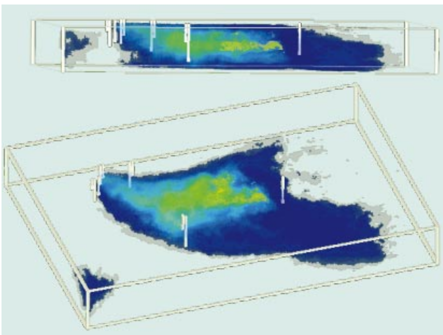

Fig. 6. ParFlow is being used to study the effect of pumping on plume migration at the Ajax site.

investigations requires the power of high performance computing and the efficiency of modern numerical methods.

Enabling Computational Technologies

Tera-scale scientific simulations require scalable numerical methods and flexible code frameworks. CASC is conducting research in both areas. We are promulgating our expertise in differential equations via the parallel PVODE package (Figure 7). Recently, we developed a fast and scalable multigrid preconditioned conjugate gradient solver for modeling groundwater flow (Figure 8), and we are currently working with ASCI code groups to modify this technology for application to radiation diffusion.

In the area of code frameworks, we are developing a parallel adaptive mesh refinement (AMR) code infrastructure for applications in materials science (Figure 9), groundwater flow modeling, and neutron transport. The design and implementation of efficient communication primitives for scientific applications (Figure 10) are critical to these efforts.

External Collaborations

In addition to our internal programmatic collaborations, CASC is also collaborating with colleagues from academia, industry, and other federal laboratories on a variety of applied research topics. For example, we are teaming with Cray Research, Inc. and Digital Equipment Corporation to integrate our numerical algorithms into their mathematical libraries.

We have an active visitor and seminar program, as well as a summer program for undergraduate and graduate students. This university outreach is an essential ingredient to CASC's long term vitality and success.

Computing Resources

LLNL is home to the ASCI Blue Pacific massively parallel computer. When fully configured in 1999, this machine will consist of 512 8-processor nodes, with an aggregate of more than 2 TB of memory. This SMP cluster will be capable of 3-TF sustained performance.

LLNL is also working with the Digital Equipment Corporation to deploy a cluster of Alpha-based SMPs as part of the Laboratory's Multiprogrammatic and Institutional Computing Initiative. The initial configuration will boast a peak of nearly 100 GF and have more than 45 GB of memory. Visualization expertise is available from LC's Visualization Laboratory.

For additional information on CASC's research efforts, or if you are interested in a visiting, career, or postdoctoral position, please contact Steven Ashby, Director, sfashby@llnl.gov.

You also are welcome to visit our Web site (www.llnl.gov/CASC).

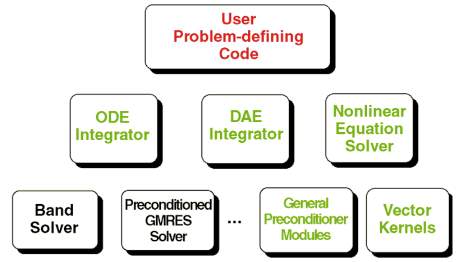

Fig. 7. PVODE, our parallel solver for nonlinear and differential equations, has a modular and extensible design.

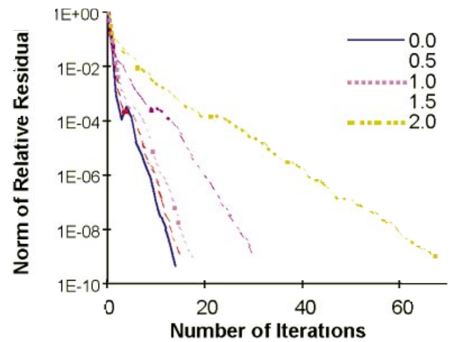

Fig. 8. Our multigrid preconditioned conjugate gradient solver is 100 times faster than competing linear solvers.

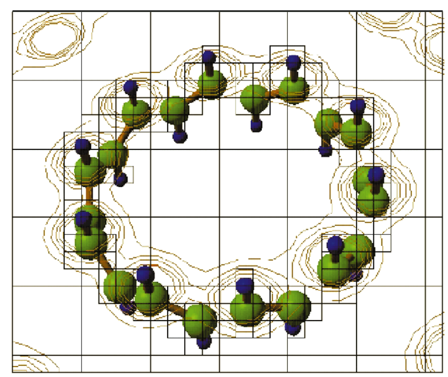

Fig. 9. Adaptive mesh refinement technology is used to focus computational effort where it is most needed.

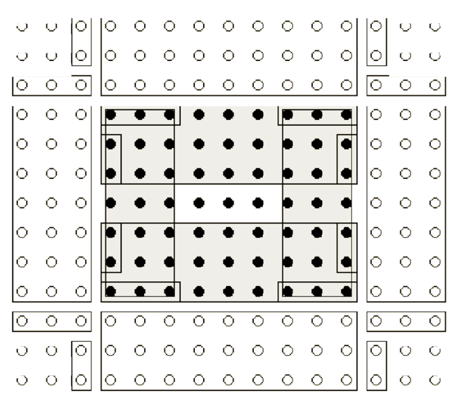

Fig. 10. Our AMPS communications layer allows the applications developer to code in terms of stencil operations.

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